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## Ground-state magnetization curve of a generalized spin-1/2 ladder

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Employing a method of exact diagonalization for finite-size systems, we investigate the magnetization curve in the ground state of an antiferromagnetic spin-1/2 ladder with additional exchange interactions on diagonal bonds, which is equivalent to an antiferromagnetic spin-1/2 chain with bond-alternating nearest-neighbor and uniform next-nearest-neighbor interactions. It is found that a half-plateau appears in the magnetization curve in a certain range of the interaction constants. This result is discussed in connection with the necessary condition for the appearance of the plateau, recently given by Oshikawa et al.

Key Words: ground-state magnetization curve, generalized spin-1/2 ladder, spin-1/2 chain with competing interactions, half-plateau

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There has been a considerable current interest in the study of quantum spin systems with competing interactions, which exhibit a variety of fascinating phenomena originating from frustration and quantum fluctuation. In this paper we investigate the magnetization curve in the ground state of an antiferromagnetic spin-1/2 ladder with additional exchange interactions on diagonal bonds. We express the Hamiltonian describing this system in an external magnetic field as

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_Z,$$

$$\mathcal{H}_0 = (1 + \alpha) \sum_{\ell=1}^{N/2} \vec{S}_{1,\ell} \cdot \vec{S}_{2,\ell} + J \sum_{j=1}^2 \sum_{\ell=1}^{N/2} \vec{S}_{j,\ell} \cdot \vec{S}_{j,\ell+1}$$
(1a)

+ 
$$(1 - \alpha) \sum_{\ell=1}^{N/2} \vec{S}_{1,\ell} \cdot \vec{S}_{2,\ell+1}$$
, (1b)

$$\mathcal{H}_{Z} = -H \sum_{j=1}^{2} \sum_{\ell=1}^{N/2} S_{j,\ell}^{z}, \qquad (1c)$$

where  $\vec{S}_{j,\ell}$  is the spin-1/2 operator at the jth leg and the  $\ell$ th rung;  $1+\alpha$  and  $1-\alpha$  ( $0.0 \le \alpha \le 1.0$ ) are, respectively, the interaction constants between neighboring spins along the rung and diagonal bonds; J ( $J \ge 0.0$ ) is the interaction constant between neighboring spins along the leg bond; H ( $H \ge 0.0$ ) is the magnitude, in an appropriate unit, of the magnetic field applied along the z-axis; N is the total number of spins in the system and is assumed to be a multiple of four. We impose periodic boundary conditions ( $\vec{S}_{j,N+1} \equiv \vec{S}_{j,1}$ ). It should be noted that this system is equivalent to an antiferromagnetic spin-1/2 chain with both bond-alternating nearest-neighbor interactions, the interaction constants being  $1+\alpha$  and  $1-\alpha$ , and uniform next-nearest-neighbor interactions, the interaction constant being J, which compete with each other.

The ground-state [1] and thermodynamic [2-4] properties of the system in the case of  $\alpha = 0.0$  and H = 0.0 have been studied extensively. In particular, it has been found that as the value of J increases, the phase transition from the massless spin-fluid phase to the massive dimer phase occurs at  $J = J_c \sim 0.2412$  in the ground state [4-6]. As is well known, the exact ground-state magnetization curve in the case of  $\alpha = J = 0.0$  has been obtained by Griffiths [7]. The ground-state magnetization curves in the case of  $\alpha = 0.0$  [8] and in the case of J = 0.0 [9] have also been numerically calculated for various values of J and  $\alpha$ , respectively.

Obtaining the ground-state magnetization curve of the present system, we employ Sakai and Takahashi's method [10], by the use of which they have discussed the ground-state magnetization curve for a uniform spin-1 chain. The outline of this method, which is based on a method of exact diagonalization for finite-size systems combined with the conformal field theory, can be summarized as follows. Let  $E_0(N, M)$  be the lowest-energy eigenvalue, within the subspace determined by the value  $M = \sum_{j=1}^{2} \sum_{\ell=1}^{N/2} S_{j,\ell}^z (=0, 1, \dots, N/2)$ , of the Hamiltonian  $\mathcal{H}_0$  for a given N. Then, the conformal field theory predicts that, if the state with the energy  $E_0(N, M)$  is massless, the asymptotic behavior of  $E_0(N, M)$  in the thermodynamic  $(N \to \infty)$  limit has the form [11]

$$\frac{E_0(N,M)}{N} \sim \varepsilon(m) - C(m) \frac{1}{N^2} \qquad (N \to \infty)$$
 (2)

with  $m \equiv M/N$ , where  $\varepsilon(m)$  is the lowest energy per spin for a given m in the thermodynamic limit and C(m) is a positive constant which is proportional to the product of the central charge and the sound velocity. Minimizing with respect to m the total energy,  $\varepsilon_{\text{tot}} = \varepsilon(m) - Hm$ , per spin of the system described by the Hamiltonian  $\mathcal{H}$ , we can obtain the equation which relates

the ground-state magnetization  $\langle m \rangle$  per spin in the thermodynamic limit with H as

$$\varepsilon'(\langle m \rangle) = H . \tag{3}$$

From Eq. (2) we can derive

$$\Delta E_0(N; M, M - 1) \sim \varepsilon'(m_{-0}) - \frac{1}{2}\varepsilon''(m_{-0})\frac{1}{N} \qquad (N \to \infty) , \quad (4a)$$

$$\Delta E_0(N; M+1, M) \sim \varepsilon'(m_{+0}) + \frac{1}{2}\varepsilon''(m_{+0})\frac{1}{N} \qquad (N \to \infty) , \quad (4b)$$

where  $\Delta E_0(N; M, M-1) \equiv E_0(N, M) - E_0(N, M-1)$ . The essential point of Sakai and Takahashi's method [10] is that as far as the massless states are concerned, Eqs. (4a,b) hold when N is sufficiently large, and thus the value  $H = \varepsilon'(m)$  [see Eq. (3)] of the magnetic field for a given m (0 < m < 1/2) can be estimated by making an extrapolation which uses these equations to be  $H = \varepsilon'(m_{-0}) = \varepsilon'(m_{+0})$ . For the estimation of  $H_{c0} \equiv \varepsilon'(0)$ , which is the critical field at which  $\langle m \rangle$  starts to increase from zero in the ground-state magnetization curve, we apply Shanks' transformation [12] to the sequences  $\{\Delta E_0(N;1,0)\}$ , following Sakai and Takahashi's procedure [13]. Furthermore, the saturation field  $H_s \equiv \varepsilon'(1/2)$  can be obtained analytically, since it is straightforward to diagonalize the Hamiltonian  $\mathcal{H}_0$  within the M = (N/2) - 1 subspace; it is given by  $H_s = \text{Max}(2, 1 + 2J + \alpha)$  in the present case. Recently, we have successfully applied the method to the case of an antiferromagnetic spin-1 chain with bond-alternating nearest-neighbor interactions and uniaxial single-ion-type anisotropy [14].

We obtain the ground-state magnetization curve in the thermodynamic limit for  $J=0.1,\ 0.2,\ 0.3,\$ and  $0.4,\$ for each of which various values of  $\alpha$  are chosen. In the calculation we numerically diagonalize the Hamiltonian  $\mathcal{H}_0$ , using the computer program package KOBEPACK/S [15], to calculate  $E_0(N,M)$  for  $N=8,\ 12,\ \cdots,\ 24$ . Then, we can make the analysis for m = 1/12, 1/8, 1/6, 1/4, 1/3, 3/8,and 5/12. Our calculation shows that both  $\Delta E_0(N; M+1, M)$  and  $\Delta E_0(N; M, M-1)$  are almost linear functions of 1/N at least for m = 1/8 and 3/8 in accordance with the forms given by Eqs. (4a,b). The values of  $\varepsilon'(m_{-0})$  and  $\varepsilon'(m_{+0})$  for these m's can thus be estimated. In a similar way we estimate  $\varepsilon'(m_{-0})$  and  $\varepsilon'(m_{+0})$  for m=1/12, 1/6, 1/3, and 5/12, assuming Eqs. (4a,b), although only two data are available. All the obtained results show that  $\varepsilon'(m_{-0})$  and  $\varepsilon'(m_{+0})$ coincide with each other within the numerical error. For m = 1/4, on the other hand, Eqs. (4a, b) do or do not hold depending upon the values of  $\alpha$  and J. The case where Eqs. (4a, b) do not hold is the case where the state with m = 1/4 is massive and therefore  $\varepsilon'(1/4_{-0})$  is smaller than  $\varepsilon'(1/4_{+0})$ . This means that, in the magnetization curve, there appears the half  $(\langle m \rangle = 1/4)$ -plateau with the critical field  $H_{c1} \equiv \varepsilon'(1/4_{-0})$  at which the plateau starts and that  $H_{c2} \equiv \varepsilon'(1/4_{+0})$  at which it ends. We estimate the former and latter critical fields by applying Shanks' transformation [12] to the sequences  $\{\Delta E_0(N; N/4, N/4-1)\}\$  and  $\{\Delta E_0(N; N/4+1, N/4)\}$ , respectively.

We find that the half-plateau appears in the magnetization curve when  $0.5 \lesssim \alpha \lesssim 0.95$  for J=0.1, when  $0.2 \lesssim \alpha \lesssim 0.85$  for J=0.2, when  $0.0 \lesssim \alpha \lesssim 0.8$  for J=0.3, and when  $0.0 < \alpha \lesssim 0.75$  for J=0.4. As an example, we depict in Fig. 1 the magnetization curve with the half-plateau, obtained for J=0.2 and  $\alpha=0.5$ . Plotting versus  $\alpha$  the critical fields  $H_{c0}$ ,  $H_{c1}$ , and  $H_{c2}$  as well as the saturation field  $H_s$ , we can draw the ground-state phase diagram on the H versus  $\alpha$  plane; the result for J=0.2 is shown in Fig. 2.

We also calculate numerically the eigenfunctions of the lowest- and second-lowest-energy states within the M=N/4 subspace for the finite-N systems, and find that at least for a set of J and  $\alpha$  giving the plateau,

the lowest-energy state for M = N/4 in the thermodynamic limit is doubly degenerate, one of the eigenfunctions of which has the periodicity n = 4 (in units of the lattice constant) concerning the translational symmetry. This result is consistent with the necessary condition  $n(S - \langle m \rangle) = \text{integer}$  for the appearance of the plateau with the magnetization  $\langle m \rangle$  (S is the magnitude of spins), which has recently been given by Oshikawa, Yamanaka, and Affleck [16]. Finally, it should be noted that very recently Totsuka [17] has clarified in an excellent way the mechanism for the appearance of the plateau in the present system, using a bosonization technique. According to this work, it becomes clear that the next-nearest-neighbor interaction plays a crucial role in the appearance of the plateau.

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## **Figure Captions**

Fig. 1. Ground-state magnetization curve in the thermodynamic limit obtained for J=0.2 and  $\alpha=0.5$ . The closed circles show plots of  $\langle m \rangle$  versus  $H=\varepsilon'(\langle m \rangle)$ . The solid lines are guides to the eye.

Fig. 2 Ground-state phase diagram on the H versus  $\alpha$  plane in the thermodynamic limit for J=0.2. The closed circles show plots versus  $\alpha$  of the critical fields  $H_{c0}$ ,  $H_{c1}$ , and  $H_{c2}$  and also of the saturation field  $H_s$ . The solid lines are guides to the eye. The magnetization  $\langle m \rangle$  is given by  $\langle m \rangle = 0$ , 1/4, and 1/2 in the regions A, B, and C, respectively. In the remaining region  $\langle m \rangle$  increases continuously as H increases.

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